



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 10:36 AM JST

PDB ID : 23VK / pdb_000023vk
Title : Crystal structure of full-length of APS kinase from Entamoeba histolytica
Authors : Hatanaka, R.; Yuasa, H.; Inoguchi, A.; Matsui, H.; Osumi, Y.; Mi-ichi, F.; Kishikawa, J.; Shiba, T.
Deposited on : 2026-02-20
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

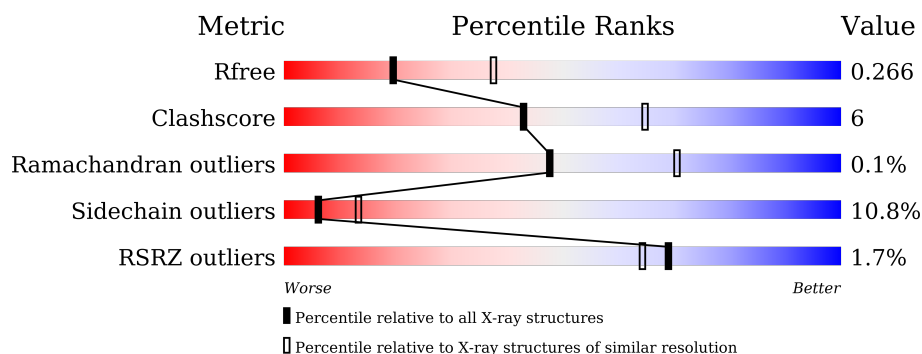
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	
1	C	500	
1	D	500	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14098 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called adenylyl-sulfate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3519	2243	599	664	13			
1	B	451	Total	C	N	O	S	0	0	0
			3513	2240	598	662	13			
1	C	450	Total	C	N	O	S	0	0	0
			3506	2235	597	661	13			
1	D	453	Total	C	N	O	S	0	0	0
			3527	2249	600	665	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0A5K1U9J0
A	-21	ASN	-	expression tag	UNP A0A5K1U9J0
A	-20	HIS	-	expression tag	UNP A0A5K1U9J0
A	-19	LYS	-	expression tag	UNP A0A5K1U9J0
A	-18	VAL	-	expression tag	UNP A0A5K1U9J0
A	-17	HIS	-	expression tag	UNP A0A5K1U9J0
A	-16	HIS	-	expression tag	UNP A0A5K1U9J0
A	-15	HIS	-	expression tag	UNP A0A5K1U9J0
A	-14	HIS	-	expression tag	UNP A0A5K1U9J0
A	-13	HIS	-	expression tag	UNP A0A5K1U9J0
A	-12	HIS	-	expression tag	UNP A0A5K1U9J0
A	-11	ILE	-	expression tag	UNP A0A5K1U9J0
A	-10	GLU	-	expression tag	UNP A0A5K1U9J0
A	-9	GLY	-	expression tag	UNP A0A5K1U9J0
A	-8	ARG	-	expression tag	UNP A0A5K1U9J0
A	-7	HIS	-	expression tag	UNP A0A5K1U9J0
A	-6	MET	-	expression tag	UNP A0A5K1U9J0
A	-5	GLU	-	expression tag	UNP A0A5K1U9J0
A	-4	LEU	-	expression tag	UNP A0A5K1U9J0
A	-3	GLY	-	expression tag	UNP A0A5K1U9J0
A	-2	THR	-	expression tag	UNP A0A5K1U9J0

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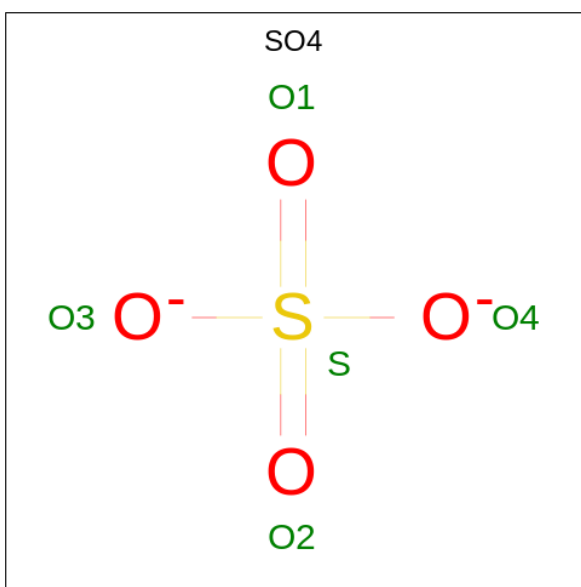
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LEU	-	expression tag	UNP A0A5K1U9J0
A	0	GLU	-	expression tag	UNP A0A5K1U9J0
B	-22	MET	-	initiating methionine	UNP A0A5K1U9J0
B	-21	ASN	-	expression tag	UNP A0A5K1U9J0
B	-20	HIS	-	expression tag	UNP A0A5K1U9J0
B	-19	LYS	-	expression tag	UNP A0A5K1U9J0
B	-18	VAL	-	expression tag	UNP A0A5K1U9J0
B	-17	HIS	-	expression tag	UNP A0A5K1U9J0
B	-16	HIS	-	expression tag	UNP A0A5K1U9J0
B	-15	HIS	-	expression tag	UNP A0A5K1U9J0
B	-14	HIS	-	expression tag	UNP A0A5K1U9J0
B	-13	HIS	-	expression tag	UNP A0A5K1U9J0
B	-12	HIS	-	expression tag	UNP A0A5K1U9J0
B	-11	ILE	-	expression tag	UNP A0A5K1U9J0
B	-10	GLU	-	expression tag	UNP A0A5K1U9J0
B	-9	GLY	-	expression tag	UNP A0A5K1U9J0
B	-8	ARG	-	expression tag	UNP A0A5K1U9J0
B	-7	HIS	-	expression tag	UNP A0A5K1U9J0
B	-6	MET	-	expression tag	UNP A0A5K1U9J0
B	-5	GLU	-	expression tag	UNP A0A5K1U9J0
B	-4	LEU	-	expression tag	UNP A0A5K1U9J0
B	-3	GLY	-	expression tag	UNP A0A5K1U9J0
B	-2	THR	-	expression tag	UNP A0A5K1U9J0
B	-1	LEU	-	expression tag	UNP A0A5K1U9J0
B	0	GLU	-	expression tag	UNP A0A5K1U9J0
C	-22	MET	-	initiating methionine	UNP A0A5K1U9J0
C	-21	ASN	-	expression tag	UNP A0A5K1U9J0
C	-20	HIS	-	expression tag	UNP A0A5K1U9J0
C	-19	LYS	-	expression tag	UNP A0A5K1U9J0
C	-18	VAL	-	expression tag	UNP A0A5K1U9J0
C	-17	HIS	-	expression tag	UNP A0A5K1U9J0
C	-16	HIS	-	expression tag	UNP A0A5K1U9J0
C	-15	HIS	-	expression tag	UNP A0A5K1U9J0
C	-14	HIS	-	expression tag	UNP A0A5K1U9J0
C	-13	HIS	-	expression tag	UNP A0A5K1U9J0
C	-12	HIS	-	expression tag	UNP A0A5K1U9J0
C	-11	ILE	-	expression tag	UNP A0A5K1U9J0
C	-10	GLU	-	expression tag	UNP A0A5K1U9J0
C	-9	GLY	-	expression tag	UNP A0A5K1U9J0
C	-8	ARG	-	expression tag	UNP A0A5K1U9J0
C	-7	HIS	-	expression tag	UNP A0A5K1U9J0
C	-6	MET	-	expression tag	UNP A0A5K1U9J0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLU	-	expression tag	UNP A0A5K1U9J0
C	-4	LEU	-	expression tag	UNP A0A5K1U9J0
C	-3	GLY	-	expression tag	UNP A0A5K1U9J0
C	-2	THR	-	expression tag	UNP A0A5K1U9J0
C	-1	LEU	-	expression tag	UNP A0A5K1U9J0
C	0	GLU	-	expression tag	UNP A0A5K1U9J0
D	-22	MET	-	initiating methionine	UNP A0A5K1U9J0
D	-21	ASN	-	expression tag	UNP A0A5K1U9J0
D	-20	HIS	-	expression tag	UNP A0A5K1U9J0
D	-19	LYS	-	expression tag	UNP A0A5K1U9J0
D	-18	VAL	-	expression tag	UNP A0A5K1U9J0
D	-17	HIS	-	expression tag	UNP A0A5K1U9J0
D	-16	HIS	-	expression tag	UNP A0A5K1U9J0
D	-15	HIS	-	expression tag	UNP A0A5K1U9J0
D	-14	HIS	-	expression tag	UNP A0A5K1U9J0
D	-13	HIS	-	expression tag	UNP A0A5K1U9J0
D	-12	HIS	-	expression tag	UNP A0A5K1U9J0
D	-11	ILE	-	expression tag	UNP A0A5K1U9J0
D	-10	GLU	-	expression tag	UNP A0A5K1U9J0
D	-9	GLY	-	expression tag	UNP A0A5K1U9J0
D	-8	ARG	-	expression tag	UNP A0A5K1U9J0
D	-7	HIS	-	expression tag	UNP A0A5K1U9J0
D	-6	MET	-	expression tag	UNP A0A5K1U9J0
D	-5	GLU	-	expression tag	UNP A0A5K1U9J0
D	-4	LEU	-	expression tag	UNP A0A5K1U9J0
D	-3	GLY	-	expression tag	UNP A0A5K1U9J0
D	-2	THR	-	expression tag	UNP A0A5K1U9J0
D	-1	LEU	-	expression tag	UNP A0A5K1U9J0
D	0	GLU	-	expression tag	UNP A0A5K1U9J0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

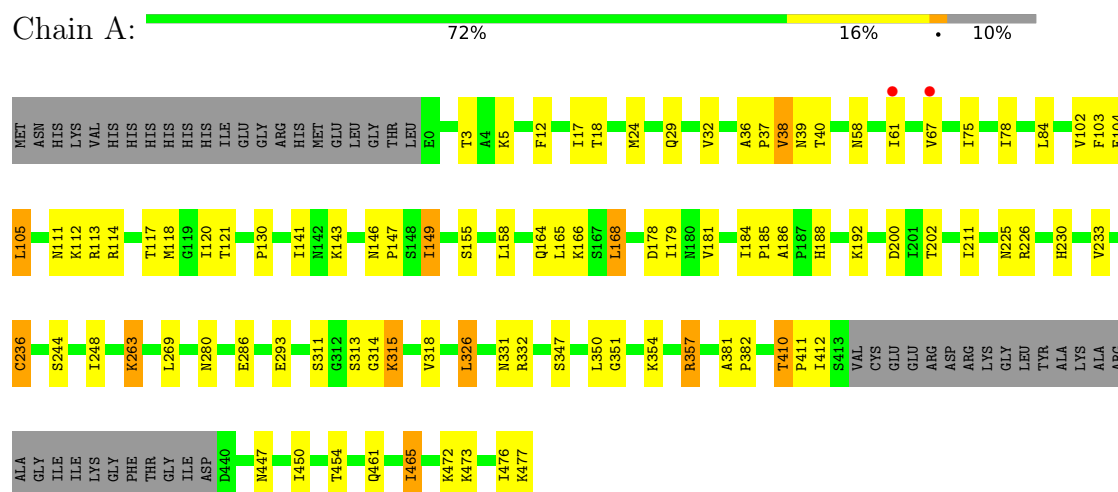
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	5	Total	O	0	0
			5	5		
3	D	2	Total	O	0	0
			2	2		

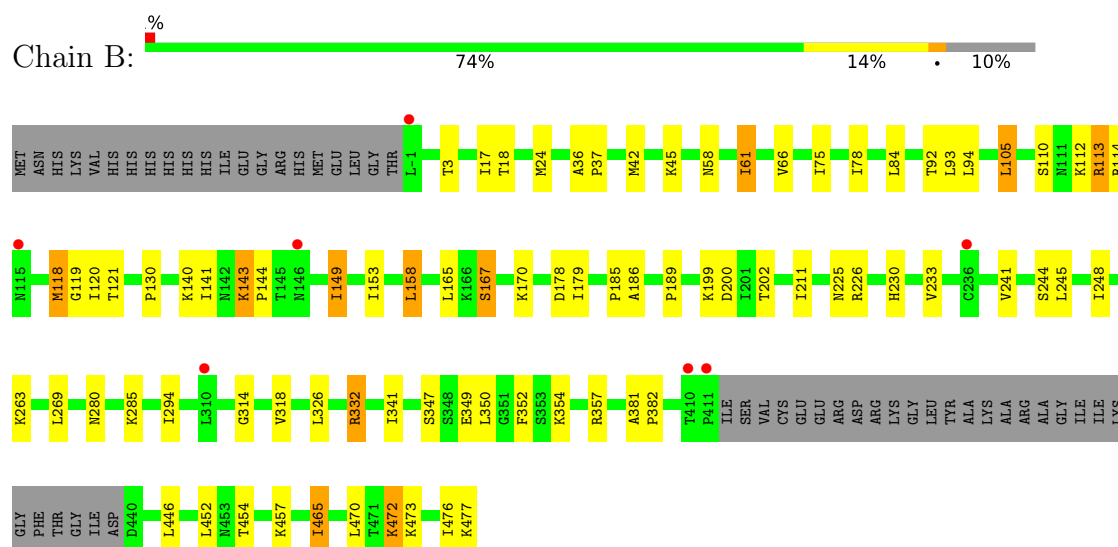
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

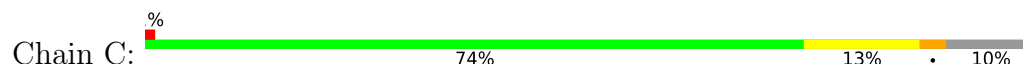
• Molecule 1: adenylyl-sulfate kinase

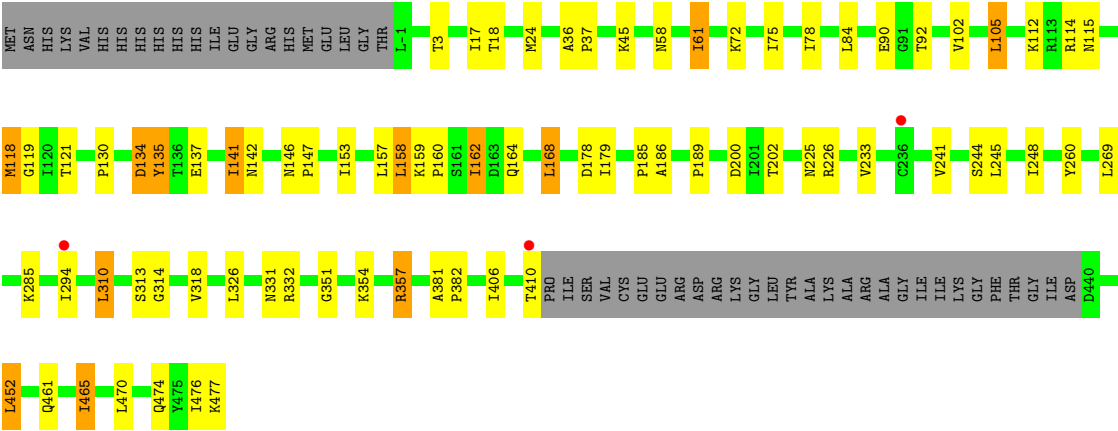


• Molecule 1: adenylyl-sulfate kinase

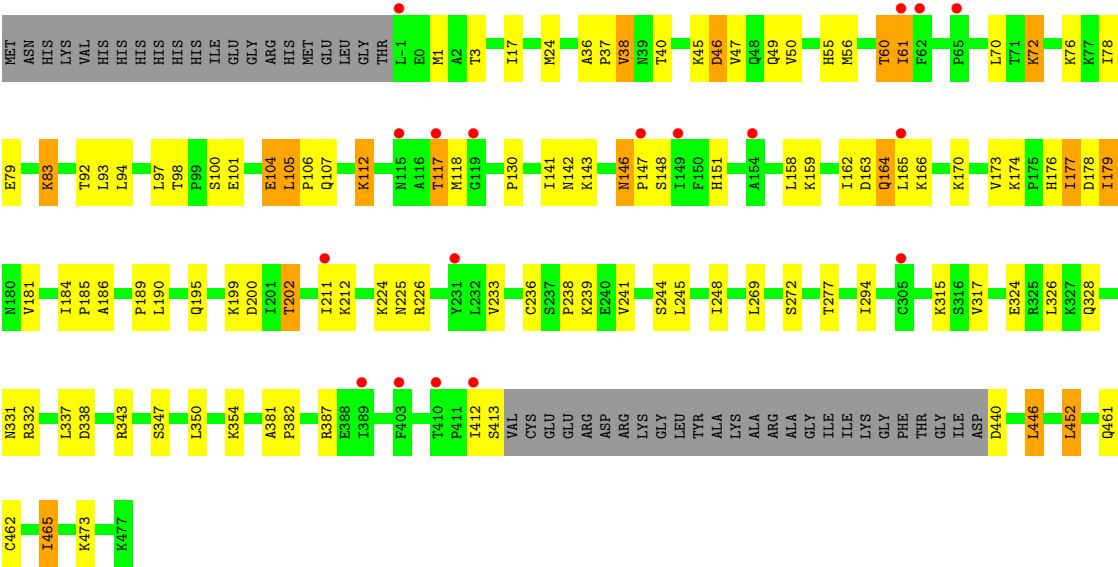


• Molecule 1: adenylyl-sulfate kinase





● Molecule 1: adenylyl-sulfate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	144.45Å 158.39Å 226.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.97-2.60) 99.3 (19.97-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.227 , 0.265 0.230 , 0.266	Depositor DCC
R_{free} test set	3995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	101.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14098	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3593	1.03	3/4873 (0.1%)
1	B	0.53	0/3587	1.04	4/4865 (0.1%)
1	C	0.52	0/3579	1.01	5/4853 (0.1%)
1	D	0.52	0/3601	1.03	3/4884 (0.1%)
All	All	0.52	0/14360	1.03	15/19475 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	THR	CA-CB-OG1	-6.76	99.47	109.60
1	B	113	ARG	NE-CZ-NH1	-6.66	114.84	121.50
1	B	332	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	C	178	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	472	LYS	CB-CG-CD	5.54	124.03	111.30
1	A	286	GLU	CB-CG-CD	5.48	121.92	112.60
1	A	178	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	178	ASP	CA-CB-CG	5.30	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	135	TYR	CB-CA-C	5.22	118.33	109.50
1	C	134	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	137	GLU	CB-CG-CD	5.08	121.24	112.60
1	D	178	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	164	GLN	N-CA-CB	5.04	117.63	110.16
1	C	135	TYR	N-CA-C	-5.03	102.08	110.17

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	332	ARG	Sidechain
1	B	113	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	332	ARG	Sidechain
1	C	332	ARG	Sidechain
1	D	332	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3519	0	3603	53	0
1	B	3513	0	3598	35	0
1	C	3506	0	3591	38	0
1	D	3527	0	3614	61	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	6	0	0	1	0
3	B	5	0	0	0	0
3	D	2	0	0	0	0
All	All	14098	0	14406	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:CYS:HB3	1:A:263:LYS:HZ3	1.30	0.96
1:A:102:VAL:HG22	1:A:120:ILE:HG22	1.50	0.94
1:A:236:CYS:HB3	1:A:263:LYS:NZ	1.83	0.93
1:D:176:HIS:NE2	1:D:202:THR:CG2	2.32	0.93
1:A:236:CYS:CB	1:A:263:LYS:NZ	2.38	0.86
1:B:42:MET:HG2	1:B:66:VAL:O	1.78	0.84
1:D:176:HIS:NE2	1:D:202:THR:HG23	1.95	0.80
1:C:36:ALA:HB2	1:C:225:ASN:OD1	1.83	0.78
1:B:452:LEU:HB3	1:B:465:ILE:HD11	1.67	0.77
1:A:236:CYS:CB	1:A:263:LYS:HZ2	1.98	0.76
1:D:36:ALA:HB3	1:D:37:PRO:HD3	1.73	0.71
1:D:61:ILE:HG23	1:D:248:ILE:HD11	1.72	0.70
1:A:36:ALA:HB3	1:A:37:PRO:HD3	1.75	0.68
1:D:55:HIS:NE2	1:D:56:MET:HE3	2.08	0.68
1:A:103:PHE:O	1:A:104:GLU:C	2.38	0.67
1:A:410:THR:HB	1:A:454:THR:HB	1.77	0.66
1:D:61:ILE:HG23	1:D:248:ILE:CD1	2.26	0.66
1:A:410:THR:HG23	1:A:411:PRO:HD3	1.78	0.65
1:A:36:ALA:HB2	1:A:225:ASN:OD1	1.96	0.65
1:C:61:ILE:HG23	1:C:248:ILE:CD1	2.27	0.65
1:B:24:MET:HE2	1:B:130:PRO:HB3	1.79	0.64
1:A:24:MET:HE2	1:A:130:PRO:HB3	1.80	0.64
1:A:102:VAL:HG22	1:A:120:ILE:CG2	2.25	0.64
1:B:36:ALA:HB3	1:B:37:PRO:HD3	1.81	0.62
1:D:179:ILE:HD11	1:D:190:LEU:HD23	1.82	0.62
1:D:36:ALA:HB2	1:D:225:ASN:OD1	1.99	0.62
1:D:104:GLU:HA	1:D:118:MET:HA	1.82	0.62
1:C:153:ILE:HD12	1:C:157:LEU:HD13	1.82	0.61
1:C:24:MET:HE2	1:C:130:PRO:HB3	1.81	0.60
1:D:176:HIS:NE2	1:D:202:THR:HG21	2.16	0.60
1:D:272:SER:HA	1:D:277:THR:HG22	1.82	0.60
1:D:83:LYS:HD3	1:D:98:THR:OG1	2.01	0.60
1:A:236:CYS:CB	1:A:263:LYS:HZ3	2.02	0.60
1:C:36:ALA:HB3	1:C:37:PRO:HD3	1.83	0.59
1:A:146:ASN:HB2	1:A:147:PRO:HD3	1.82	0.59
1:A:450:ILE:CG2	1:A:465:ILE:HD11	2.33	0.59
1:D:105:LEU:HD12	1:D:106:PRO:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:CB	1:B:465:ILE:HD11	2.33	0.58
1:A:211:ILE:HD12	1:A:236:CYS:SG	2.43	0.58
1:C:146:ASN:HB3	1:C:147:PRO:HD3	1.87	0.57
1:A:236:CYS:HB2	1:A:263:LYS:HZ2	1.67	0.56
1:D:24:MET:HE2	1:D:130:PRO:HB3	1.87	0.56
1:B:153:ILE:HD11	1:B:179:ILE:CD1	2.35	0.56
1:C:61:ILE:HG23	1:C:248:ILE:HD13	1.88	0.56
1:A:313:SER:HA	1:A:410:THR:CG2	2.35	0.55
1:C:36:ALA:HB3	1:C:37:PRO:CD	2.37	0.55
1:C:351:GLY:O	1:C:357:ARG:NH2	2.39	0.55
1:B:36:ALA:HB2	1:B:225:ASN:OD1	2.07	0.55
1:A:236:CYS:HB2	1:A:263:LYS:NZ	2.17	0.55
1:C:36:ALA:HB2	1:C:225:ASN:CG	2.32	0.55
1:D:36:ALA:HB2	1:D:225:ASN:CG	2.32	0.54
1:A:450:ILE:HG21	1:A:465:ILE:HD11	1.90	0.54
1:A:351:GLY:O	1:A:357:ARG:NH2	2.41	0.54
1:C:159:LYS:HB3	1:C:160:PRO:HD3	1.90	0.54
1:D:315:LYS:HG3	2:D:501:SO4:O2	2.08	0.53
1:D:36:ALA:HB3	1:D:37:PRO:CD	2.39	0.53
1:D:272:SER:HA	1:D:277:THR:CG2	2.38	0.53
1:D:50:VAL:HG22	1:D:55:HIS:HA	1.91	0.53
1:A:36:ALA:HB3	1:A:37:PRO:CD	2.38	0.53
1:D:189:PRO:HG2	1:D:294:ILE:HG13	1.90	0.53
1:A:38:VAL:HG12	1:A:40:THR:O	2.09	0.52
1:C:61:ILE:HG23	1:C:248:ILE:HD11	1.89	0.52
1:D:181:VAL:HA	1:D:184:ILE:CG2	2.40	0.52
1:B:36:ALA:HB3	1:B:37:PRO:CD	2.39	0.52
1:D:244:SER:O	1:D:248:ILE:HG12	2.10	0.52
1:D:151:HIS:HB3	1:D:177:ILE:HD13	1.91	0.52
1:B:244:SER:O	1:B:248:ILE:HG12	2.09	0.52
1:B:61:ILE:HD12	1:B:61:ILE:H	1.74	0.52
1:C:331:ASN:HB3	1:D:294:ILE:CD1	2.40	0.52
1:A:211:ILE:HD11	1:A:263:LYS:HA	1.92	0.51
1:B:105:LEU:HD13	1:B:119:GLY:N	2.25	0.51
1:D:412:ILE:O	1:D:413:SER:C	2.53	0.51
1:B:202:THR:HG21	1:B:226:ARG:HH22	1.74	0.51
1:C:202:THR:HG21	1:C:226:ARG:HH22	1.75	0.51
1:A:103:PHE:O	1:A:103:PHE:CD2	2.64	0.51
1:A:202:THR:HG21	1:A:226:ARG:HH22	1.76	0.51
1:D:179:ILE:HD11	1:D:190:LEU:CD2	2.41	0.51
1:C:134:ASP:O	1:D:328:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:HD13	1:C:119:GLY:N	2.24	0.51
1:D:211:ILE:C	1:D:211:ILE:HD12	2.36	0.51
1:A:410:THR:N	1:A:411:PRO:CD	2.74	0.51
1:C:189:PRO:HG2	1:C:294:ILE:HG13	1.93	0.51
1:C:244:SER:O	1:C:248:ILE:HG12	2.11	0.50
1:D:47:VAL:CG1	1:D:106:PRO:HG2	2.41	0.50
1:D:49:GLN:HB3	1:D:55:HIS:O	2.11	0.50
1:D:72:LYS:H	1:D:72:LYS:CD	2.24	0.50
1:A:181:VAL:HA	1:A:184:ILE:CG2	2.42	0.50
1:B:352:PHE:HE2	1:C:102:VAL:HG23	1.76	0.50
1:B:167:SER:O	1:B:170:LYS:HG3	2.12	0.49
1:B:189:PRO:HG2	1:B:294:ILE:HG13	1.94	0.49
1:D:46:ASP:CG	1:D:56:MET:HE2	2.37	0.49
1:B:42:MET:O	1:B:121:THR:CG2	2.61	0.49
1:D:55:HIS:HB3	1:D:60:THR:N	2.26	0.49
1:D:105:LEU:HB3	1:D:117:THR:O	2.12	0.49
1:B:314:GLY:O	1:B:318:VAL:HG12	2.13	0.48
1:A:36:ALA:HB2	1:A:225:ASN:CG	2.37	0.48
1:A:314:GLY:O	1:A:318:VAL:HG12	2.14	0.48
1:B:153:ILE:HD11	1:B:179:ILE:HD13	1.96	0.48
1:D:446:LEU:HD13	1:D:446:LEU:N	2.29	0.47
1:D:105:LEU:O	1:D:105:LEU:HG	2.13	0.47
1:C:314:GLY:O	1:C:318:VAL:HG12	2.15	0.47
1:D:158:LEU:HD11	1:D:269:LEU:HD11	1.96	0.47
1:A:315:LYS:HG3	2:A:501:SO4:O2	2.14	0.47
1:B:158:LEU:HD21	1:B:269:LEU:HD11	1.96	0.47
1:D:146:ASN:O	1:D:148:SER:HB2	2.15	0.47
1:D:452:LEU:HD11	1:D:462:CYS:SG	2.55	0.47
1:D:338:ASP:HB2	1:D:381:ALA:H	1.80	0.47
1:A:331:ASN:HB3	1:B:294:ILE:HD11	1.97	0.46
1:B:105:LEU:HD13	1:B:118:MET:C	2.40	0.46
1:B:61:ILE:HD12	1:B:61:ILE:N	2.30	0.46
1:C:406:ILE:HG22	1:C:452:LEU:HD11	1.98	0.46
1:D:315:LYS:NZ	1:D:382:PRO:O	2.40	0.46
1:C:105:LEU:HD13	1:C:118:MET:C	2.40	0.46
1:A:315:LYS:HG3	2:A:501:SO4:S	2.55	0.46
1:D:159:LYS:HE3	1:D:163:ASP:OD1	2.16	0.46
1:A:114:ARG:NH2	3:A:601:HOH:O	2.49	0.46
1:C:406:ILE:CG2	1:C:452:LEU:HD11	2.46	0.46
1:D:272:SER:HB2	1:D:277:THR:HG23	1.98	0.46
1:A:146:ASN:CB	1:A:147:PRO:HD3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ALA:N	1:B:382:PRO:HD3	2.32	0.45
1:C:141:ILE:C	1:C:141:ILE:HD12	2.41	0.45
1:C:331:ASN:HB3	1:D:294:ILE:HD11	1.98	0.45
1:C:202:THR:HG21	1:C:226:ARG:NH2	2.31	0.45
1:D:238:PRO:O	1:D:241:VAL:HG22	2.16	0.45
1:C:310:LEU:H	1:C:310:LEU:HD13	1.81	0.45
1:B:24:MET:HE3	1:B:94:LEU:HD11	1.99	0.45
1:D:381:ALA:N	1:D:382:PRO:HD3	2.31	0.45
1:A:381:ALA:N	1:A:382:PRO:HD3	2.32	0.45
1:B:78:ILE:HD11	1:B:120:ILE:HD12	1.98	0.45
1:A:202:THR:HG21	1:A:226:ARG:NH2	2.32	0.45
1:B:202:THR:HG21	1:B:226:ARG:NH2	2.31	0.45
1:B:78:ILE:CD1	1:B:120:ILE:HD12	2.47	0.44
1:A:185:PRO:O	1:A:186:ALA:HB3	2.17	0.44
1:C:294:ILE:CD1	1:D:331:ASN:HB3	2.48	0.44
1:D:347:SER:HB2	1:D:350:LEU:HD12	2.00	0.44
1:C:164:GLN:O	1:C:168:LEU:HD22	2.18	0.44
1:B:185:PRO:O	1:B:186:ALA:HB3	2.17	0.44
1:D:185:PRO:O	1:D:186:ALA:HB3	2.18	0.44
1:A:347:SER:HB2	1:A:350:LEU:HD12	2.00	0.43
1:C:75:ILE:HA	1:C:78:ILE:HD12	2.00	0.43
1:D:146:ASN:O	1:D:147:PRO:C	2.61	0.43
1:D:211:ILE:HD13	1:D:236:CYS:SG	2.58	0.43
1:C:185:PRO:O	1:C:186:ALA:HB3	2.18	0.43
1:A:164:GLN:O	1:A:168:LEU:HD22	2.18	0.43
1:C:90:GLU:HG2	1:D:317:VAL:HG13	2.01	0.43
1:A:75:ILE:HA	1:A:78:ILE:HD12	2.01	0.43
1:B:75:ILE:HA	1:B:78:ILE:HD12	2.01	0.43
1:A:32:VAL:HG12	1:A:32:VAL:O	2.19	0.42
1:B:143:LYS:HD2	1:B:144:PRO:HD2	2.00	0.42
1:D:24:MET:HE3	1:D:94:LEU:HD11	2.01	0.42
1:A:331:ASN:HB3	1:B:294:ILE:CD1	2.50	0.42
1:A:105:LEU:HG	1:A:117:THR:C	2.44	0.42
1:C:135:TYR:CD1	1:D:328:GLN:NE2	2.88	0.42
1:A:141:ILE:HD12	1:A:226:ARG:CZ	2.50	0.42
1:A:149:ILE:HG23	1:A:230:HIS:HB2	2.00	0.42
1:A:158:LEU:HD21	1:A:269:LEU:HD11	2.02	0.42
1:D:461:GLN:O	1:D:465:ILE:HG23	2.19	0.42
1:C:158:LEU:HD21	1:C:269:LEU:HD11	2.01	0.41
1:C:381:ALA:N	1:C:382:PRO:HD3	2.34	0.41
1:D:50:VAL:CG2	1:D:55:HIS:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:O	1:A:465:ILE:HG23	2.19	0.41
1:D:38:VAL:HG12	1:D:40:THR:O	2.20	0.41
1:A:450:ILE:CG2	1:A:465:ILE:CD1	2.97	0.41
1:B:211:ILE:HD11	1:B:263:LYS:HG2	2.03	0.41
1:B:149:ILE:HG23	1:B:230:HIS:HB2	2.01	0.41
1:D:387:ARG:HD3	1:D:446:LEU:HD22	2.02	0.41
1:C:461:GLN:O	1:C:465:ILE:HG23	2.20	0.41
1:B:42:MET:CG	1:B:66:VAL:O	2.59	0.41
1:A:244:SER:O	1:A:248:ILE:HG13	2.21	0.41
1:C:158:LEU:O	1:C:162:ILE:HG23	2.21	0.41
1:C:310:LEU:O	1:C:313:SER:OG	2.35	0.40
1:D:142:ASN:OD1	1:D:142:ASN:N	2.53	0.40
1:A:12:PHE:CE1	1:D:440:ASP:HB2	2.56	0.40
1:A:188:HIS:NE2	1:A:192:LYS:HE2	2.37	0.40
1:B:347:SER:HB2	1:B:350:LEU:HD12	2.02	0.40
1:A:326:LEU:HD12	1:A:326:LEU:HA	1.97	0.40
1:D:112:LYS:HE2	1:D:112:LYS:HB2	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/500 (90%)	420 (94%)	28 (6%)	0	100	100
1	B	447/500 (89%)	426 (95%)	21 (5%)	0	100	100
1	C	446/500 (89%)	423 (95%)	23 (5%)	0	100	100
1	D	449/500 (90%)	419 (93%)	29 (6%)	1 (0%)	43	66
All	All	1790/2000 (90%)	1688 (94%)	101 (6%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	60	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/440 (91%)	360 (90%)	41 (10%)	7	15
1	B	400/440 (91%)	359 (90%)	41 (10%)	7	15
1	C	399/440 (91%)	361 (90%)	38 (10%)	8	18
1	D	402/440 (91%)	349 (87%)	53 (13%)	4	8
All	All	1602/1760 (91%)	1429 (89%)	173 (11%)	6	13

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	LYS
1	A	17	ILE
1	A	18	THR
1	A	29	GLN
1	A	38	VAL
1	A	39	ASN
1	A	58	ASN
1	A	61	ILE
1	A	67	VAL
1	A	84	LEU
1	A	105	LEU
1	A	111	ASN
1	A	112	LYS
1	A	118	MET
1	A	143	LYS
1	A	149	ILE
1	A	155	SER
1	A	165	LEU
1	A	166	LYS
1	A	168	LEU

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Mol	Chain	Res	Type
1	A	179	ILE
1	A	200	ASP
1	A	233	VAL
1	A	236	CYS
1	A	263	LYS
1	A	280	ASN
1	A	293	GLU
1	A	311	SER
1	A	315	LYS
1	A	326	LEU
1	A	354	LYS
1	A	357	ARG
1	A	410	THR
1	A	412	ILE
1	A	447	ASN
1	A	465	ILE
1	A	472	LYS
1	A	473	LYS
1	A	476	ILE
1	A	477	LYS
1	B	3	THR
1	B	17	ILE
1	B	18	THR
1	B	45	LYS
1	B	58	ASN
1	B	61	ILE
1	B	84	LEU
1	B	92	THR
1	B	93	LEU
1	B	105	LEU
1	B	110	SER
1	B	112	LYS
1	B	118	MET
1	B	140	LYS
1	B	141	ILE
1	B	143	LYS
1	B	149	ILE
1	B	158	LEU
1	B	165	LEU
1	B	167	SER
1	B	199	LYS
1	B	200	ASP

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Mol	Chain	Res	Type
1	B	233	VAL
1	B	241	VAL
1	B	245	LEU
1	B	280	ASN
1	B	285	LYS
1	B	326	LEU
1	B	341	ILE
1	B	349	GLU
1	B	354	LYS
1	B	357	ARG
1	B	446	LEU
1	B	454	THR
1	B	457	LYS
1	B	465	ILE
1	B	470	LEU
1	B	472	LYS
1	B	473	LYS
1	B	476	ILE
1	B	477	LYS
1	C	3	THR
1	C	17	ILE
1	C	18	THR
1	C	45	LYS
1	C	58	ASN
1	C	61	ILE
1	C	72	LYS
1	C	84	LEU
1	C	92	THR
1	C	105	LEU
1	C	112	LYS
1	C	114	ARG
1	C	115	ASN
1	C	118	MET
1	C	121	THR
1	C	141	ILE
1	C	142	ASN
1	C	158	LEU
1	C	162	ILE
1	C	168	LEU
1	C	179	ILE
1	C	200	ASP
1	C	233	VAL

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Mol	Chain	Res	Type
1	C	241	VAL
1	C	245	LEU
1	C	260	TYR
1	C	285	LYS
1	C	310	LEU
1	C	326	LEU
1	C	354	LYS
1	C	357	ARG
1	C	410	THR
1	C	452	LEU
1	C	465	ILE
1	C	470	LEU
1	C	474	GLN
1	C	476	ILE
1	C	477	LYS
1	D	1	MET
1	D	3	THR
1	D	17	ILE
1	D	38	VAL
1	D	45	LYS
1	D	61	ILE
1	D	70	LEU
1	D	72	LYS
1	D	76	LYS
1	D	78	ILE
1	D	79	GLU
1	D	83	LYS
1	D	92	THR
1	D	93	LEU
1	D	97	LEU
1	D	100	SER
1	D	101	GLU
1	D	104	GLU
1	D	105	LEU
1	D	107	GLN
1	D	112	LYS
1	D	117	THR
1	D	141	ILE
1	D	143	LYS
1	D	146	ASN
1	D	162	ILE
1	D	164	GLN

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Mol	Chain	Res	Type
1	D	165	LEU
1	D	166	LYS
1	D	170	LYS
1	D	173	VAL
1	D	174	LYS
1	D	177	ILE
1	D	179	ILE
1	D	195	GLN
1	D	199	LYS
1	D	200	ASP
1	D	202	THR
1	D	212	LYS
1	D	224	LYS
1	D	226	ARG
1	D	233	VAL
1	D	239	LYS
1	D	245	LEU
1	D	324	GLU
1	D	326	LEU
1	D	337	LEU
1	D	343	ARG
1	D	354	LYS
1	D	446	LEU
1	D	452	LEU
1	D	465	ILE
1	D	473	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	107	GLN
1	A	230	HIS
1	B	22	HIS
1	B	48	GLN
1	B	55	HIS
1	C	48	GLN
1	C	230	HIS
1	C	301	GLN
1	C	402	ASN
1	D	22	HIS
1	D	48	GLN

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Mol	Chain	Res	Type
1	D	111	ASN
1	D	115	ASN
1	D	146	ASN
1	D	151	HIS
1	D	447	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	501	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	A	501	-	4,4,4	0.39	0	6,6,6	0.19	0
2	SO4	B	501	-	4,4,4	0.48	0	6,6,6	0.18	0
2	SO4	D	501	-	4,4,4	0.44	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

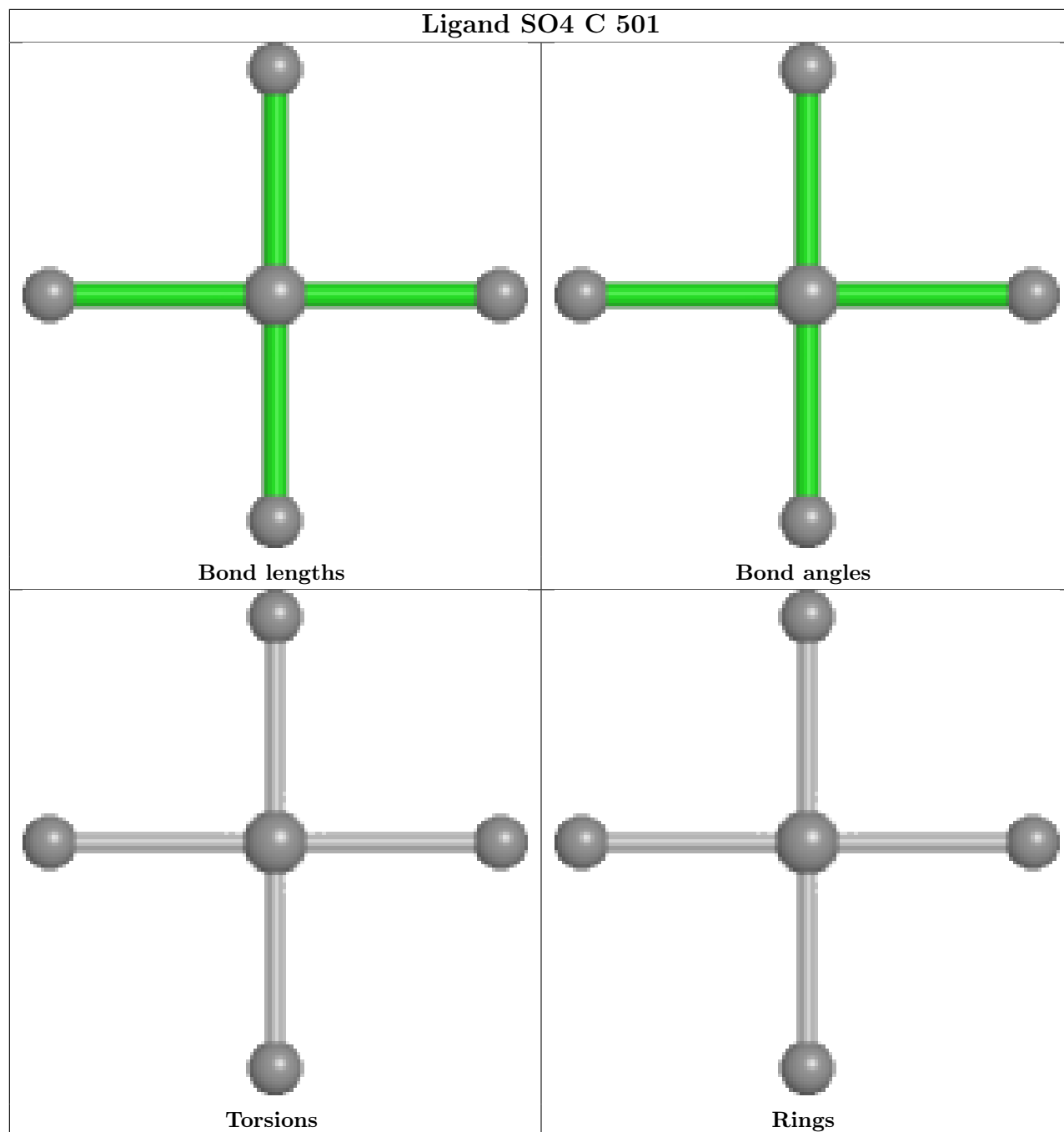
There are no torsion outliers.

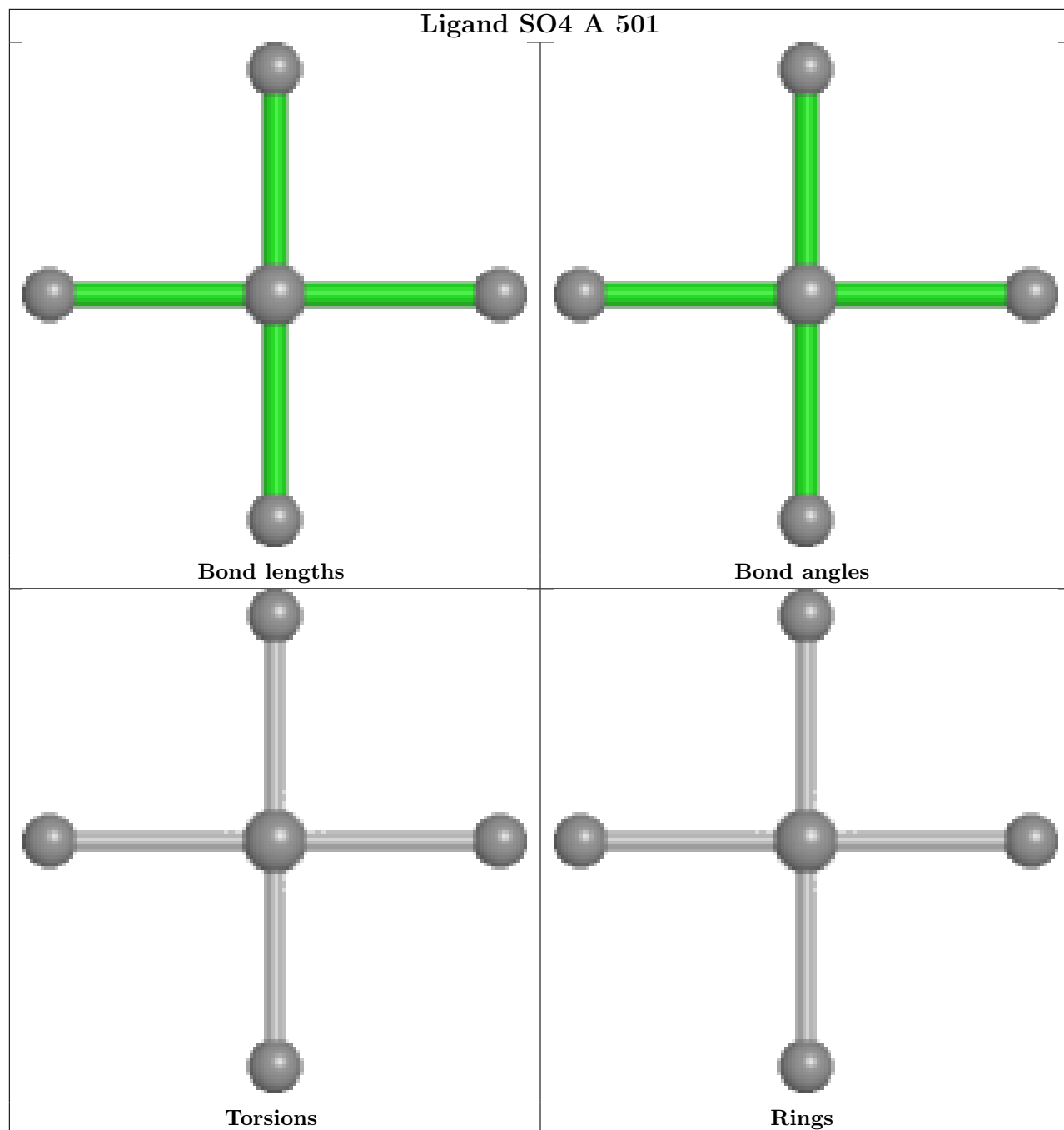
There are no ring outliers.

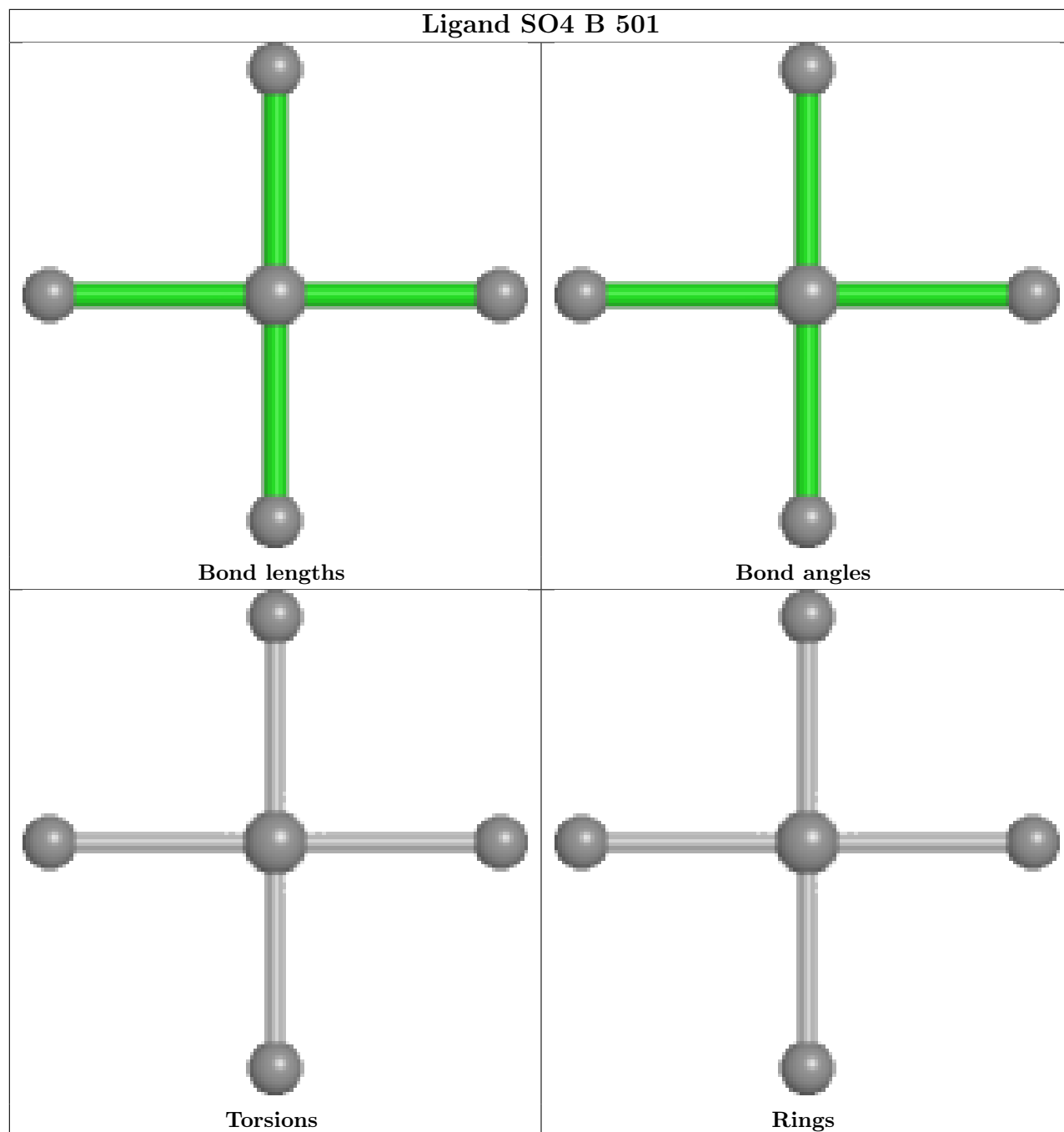
2 monomers are involved in 3 short contacts:

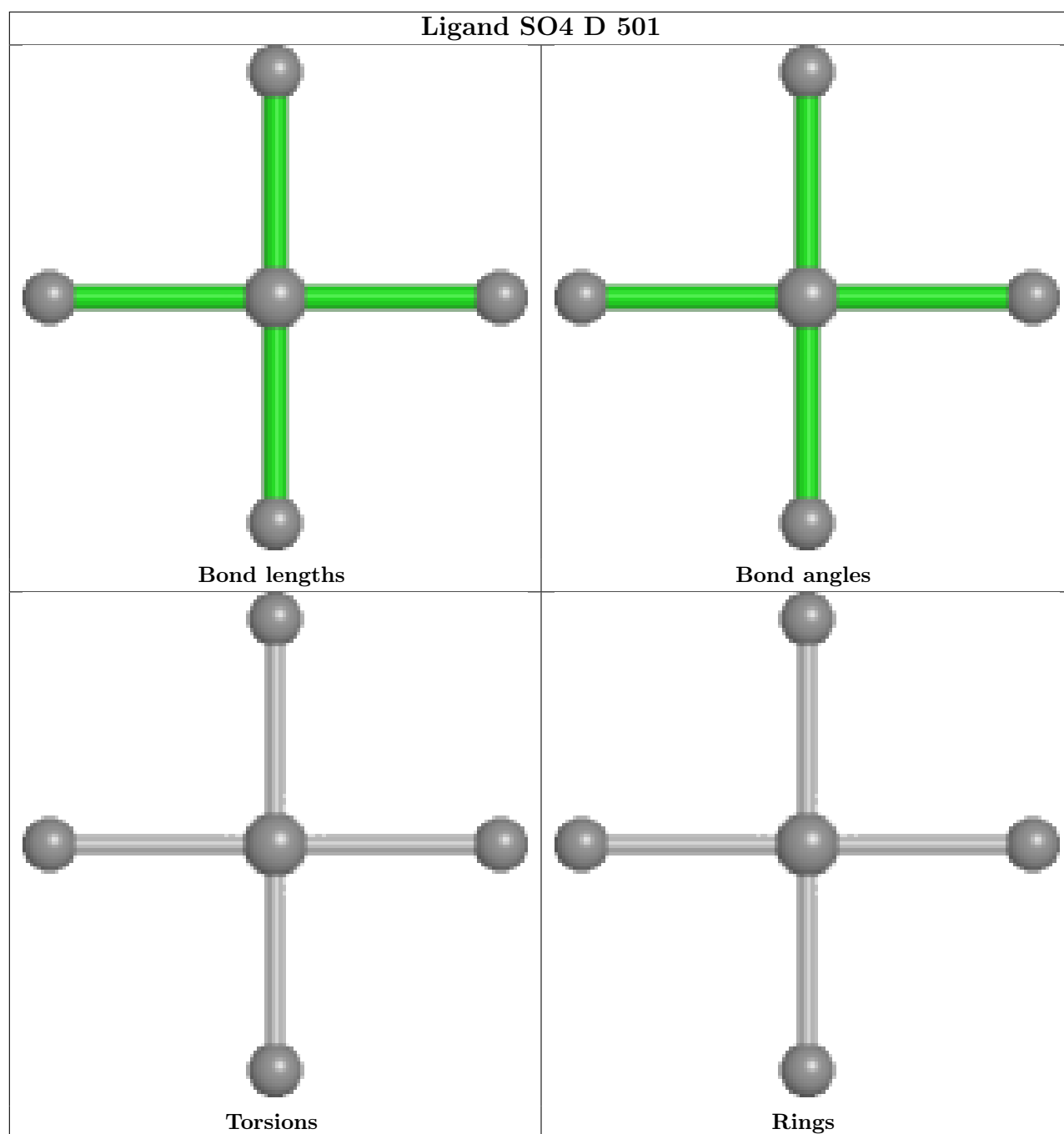
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	2	0
2	D	501	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/500 (90%)	-0.06	2 (0%) 88 86	65, 103, 147, 194	0
1	B	451/500 (90%)	-0.07	7 (1%) 70 66	58, 97, 144, 188	0
1	C	450/500 (90%)	-0.07	3 (0%) 84 82	71, 105, 144, 178	0
1	D	453/500 (90%)	0.35	18 (3%) 42 37	82, 130, 191, 234	0
All	All	1806/2000 (90%)	0.04	30 (1%) 69 64	58, 108, 168, 234	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	THR	4.0
1	B	115	ASN	3.7
1	D	305	CYS	3.6
1	D	-1	LEU	3.1
1	D	410	THR	3.0
1	D	154	ALA	2.9
1	D	147	PRO	2.8
1	C	236	CYS	2.8
1	D	61	ILE	2.7
1	D	115	ASN	2.6
1	A	61	ILE	2.6
1	B	-1	LEU	2.6
1	D	211	ILE	2.4
1	B	146	ASN	2.4
1	D	412	ILE	2.4
1	B	411	PRO	2.3
1	C	410	THR	2.3
1	C	294	ILE	2.2
1	B	236	CYS	2.2
1	D	62	PHE	2.2
1	D	231	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	117	THR	2.1
1	D	389	ILE	2.1
1	B	310	LEU	2.1
1	D	119	GLY	2.1
1	D	149	ILE	2.1
1	D	403	PHE	2.0
1	D	165	LEU	2.0
1	A	67	VAL	2.0
1	D	65	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

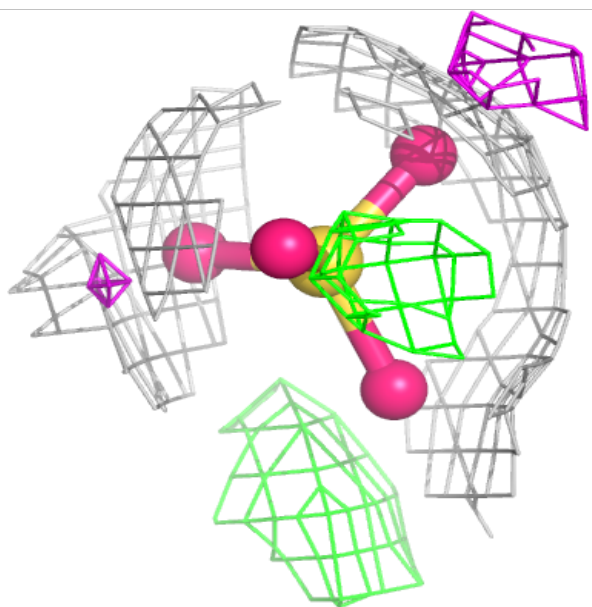
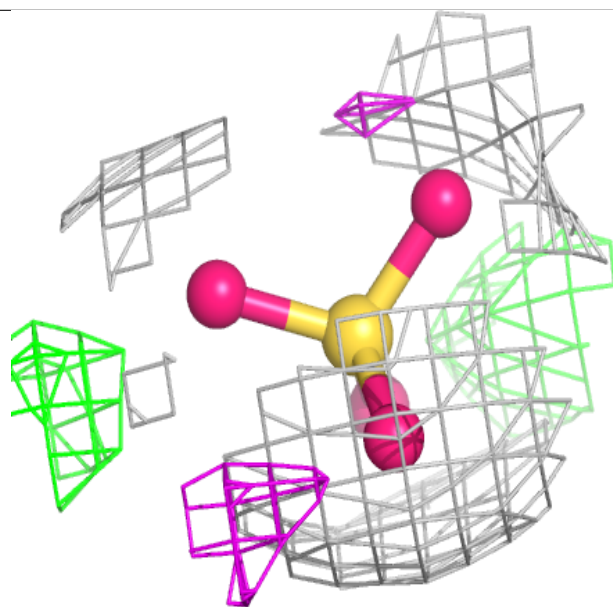
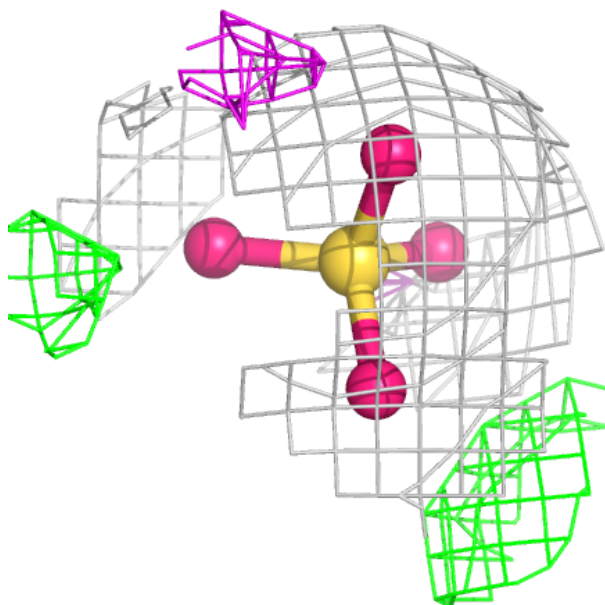
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	D	501	5/5	0.88	0.08	93,101,111,115	0
2	SO4	C	501	5/5	0.90	0.06	95,102,111,112	0
2	SO4	A	501	5/5	0.92	0.06	90,98,107,126	0
2	SO4	B	501	5/5	0.98	0.04	69,75,93,96	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

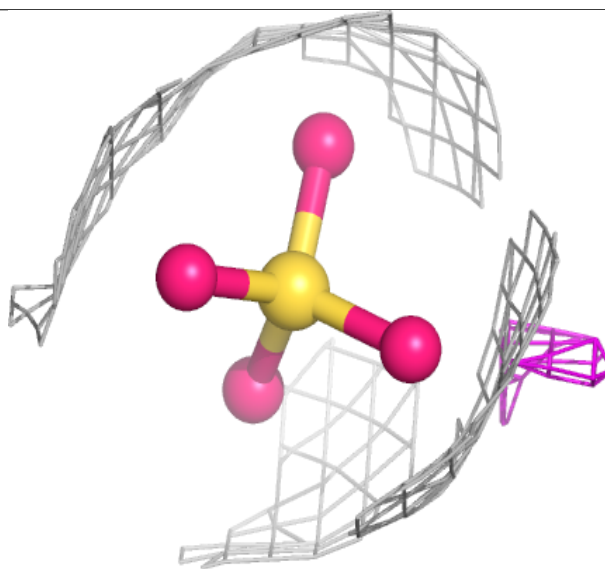
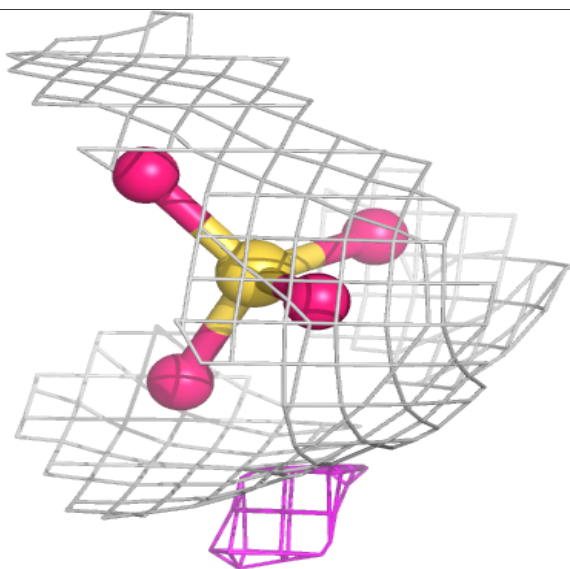
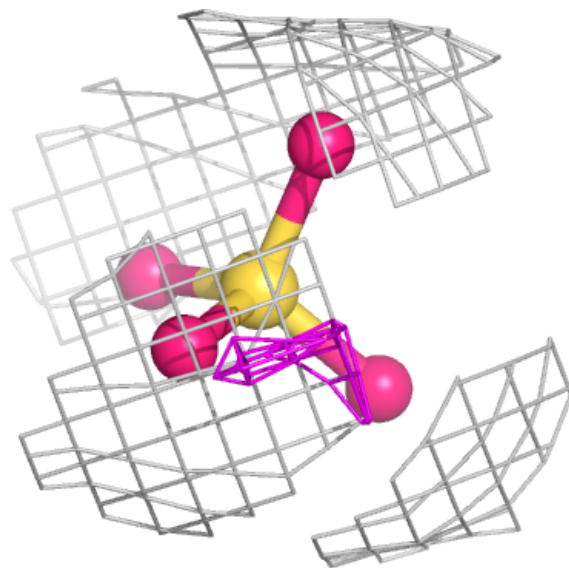
Electron density around SO4 D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



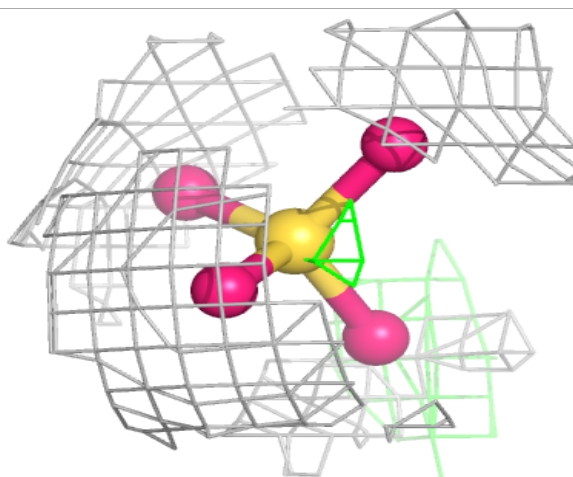
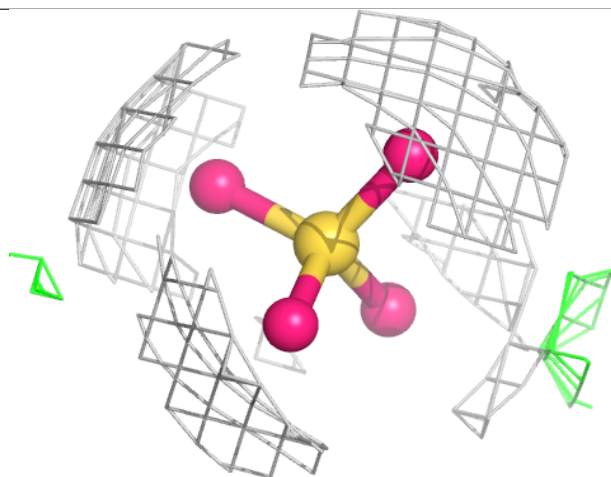
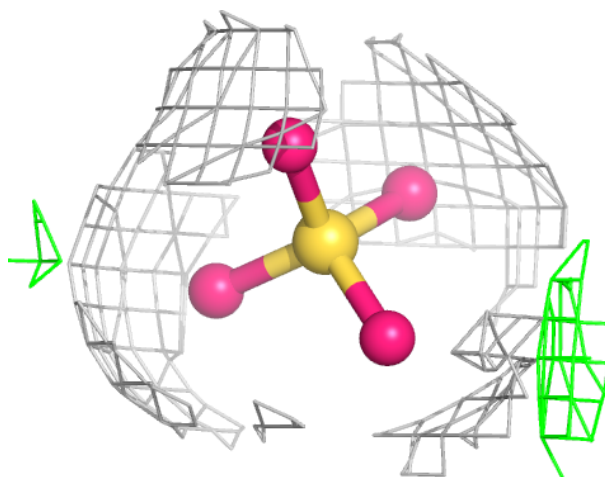
Electron density around SO4 C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



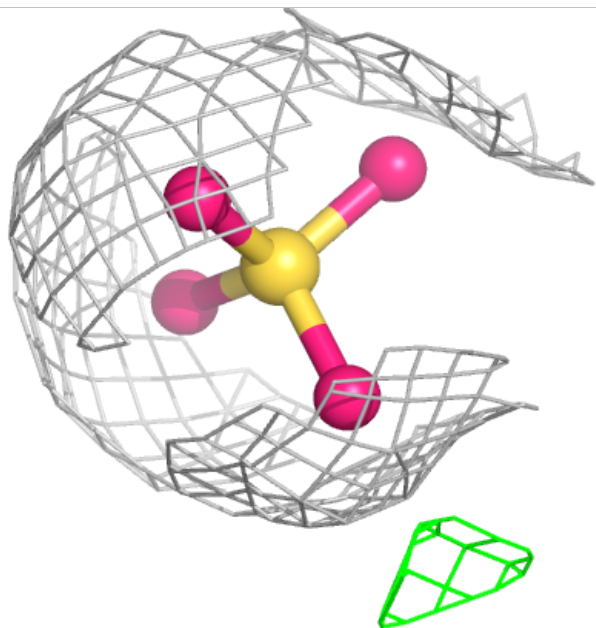
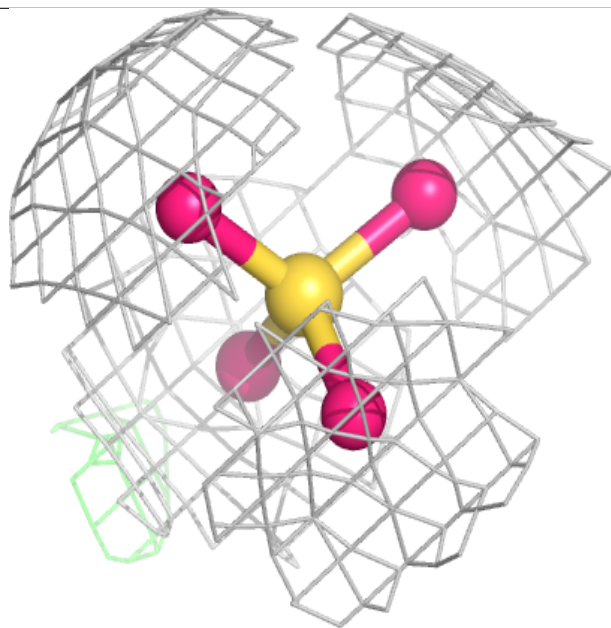
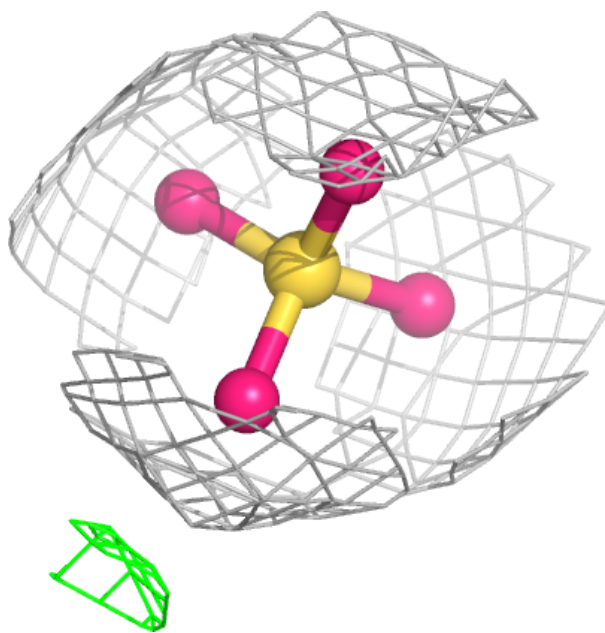
Electron density around SO4 A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.